

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU121421\
 Data File : VU046347.D
 Acq On : 14 Dec 2021 11:56
 Operator : SY/MD
 Sample : VU1214MBL01
 Misc : 5.00g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 3 Sample Multiplier: 1

Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

Filtering: 5

Sampling : 1

Min Area: 0 % of largest Peak

Start Thrs: 0.2

Max Peaks: 100

Stop Thrs : 0

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM112921WMA.M

Title : VOC Analysis

Signal : TIC: VU046347.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.604	75	82	100	rVB	76189	87096	15.26%	1.930%
2	1.922	172	181	200	rVB	57517	77319	13.55%	1.714%
3	2.575	372	384	414	rBV	123149	205064	35.94%	4.545%
4	2.800	450	454	460	rVB2	295	390	0.07%	0.009%
5	3.054	526	533	541	rVB3	735	1109	0.19%	0.025%
6	3.179	567	572	574	rBV	141	180	0.03%	0.004%
7	3.308	608	612	614	rBV	139	123	0.02%	0.003%
8	3.446	652	655	657	rBV	146	121	0.02%	0.003%
9	3.485	664	667	671	rBB	148	149	0.03%	0.003%
10	3.584	694	698	699	rBV	140	124	0.02%	0.003%
11	3.671	721	725	727	rBB	205	153	0.03%	0.003%
12	3.697	730	733	735	rBV	140	122	0.02%	0.003%
13	3.912	795	800	803	rBV	144	163	0.03%	0.004%
14	4.041	836	840	846	rBB	181	247	0.04%	0.005%
15	4.137	866	870	873	rBB	140	137	0.02%	0.003%
16	4.260	904	908	912	rBV	190	220	0.04%	0.005%
17	4.411	951	955	958	rBB	158	123	0.02%	0.003%
18	4.645	1013	1028	1072	rBV	42939	143227	25.10%	3.174%
19	4.999	1136	1138	1141	rBV	164	138	0.02%	0.003%
20	5.070	1144	1160	1180	rVV	107191	233156	40.86%	5.167%
21	5.205	1199	1202	1206	rBV	133	154	0.03%	0.003%
22	5.240	1210	1213	1216	rBB2	231	127	0.02%	0.003%
23	5.289	1225	1228	1229	rBV	262	174	0.03%	0.004%
24	5.311	1232	1235	1239	rVV2	257	277	0.05%	0.006%
25	5.334	1240	1242	1245	rVV2	213	131	0.02%	0.003%
26	5.353	1246	1248	1251	rVV	258	179	0.03%	0.004%
27	5.581	1315	1319	1321	rBB	224	130	0.02%	0.003%
28	5.633	1331	1335	1338	rBB	139	142	0.02%	0.003%
29	5.732	1344	1366	1386	rBV2	209578	570601	100.00%	12.646%
30	5.880	1409	1412	1415	rBV2	252	146	0.03%	0.003%
31	6.041	1457	1462	1467	rBB	144	188	0.03%	0.004%
32	6.112	1480	1484	1486	rBV	135	145	0.03%	0.003%
33	6.253	1514	1528	1546	rVV	179798	341625	59.87%	7.571%
34	6.424	1577	1581	1584	rBB	157	159	0.03%	0.004%
35	6.530	1611	1614	1618	rBV	376	348	0.06%	0.008%
36	6.697	1652	1666	1690	rBB	132463	258812	45.36%	5.736%

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Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

Filtering: 5

Sampling : 1

Min Area: 0 % of largest Peak

Start Thrs: 0.2

Max Peaks: 100

Stop Thrs : 0

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM112921WMA.M
 Title : VOC Analysis

37	6.941	1739	1742	1744	rBV	173	141	0.02%	0.003%
38	7.034	1768	1771	1773	rBV	169	149	0.03%	0.003%
39	7.118	1794	1797	1801	rVB	174	163	0.03%	0.004%
40	7.163	1807	1811	1815	rBB	156	144	0.03%	0.003%
41	7.192	1815	1820	1821	rBV	294	313	0.05%	0.007%
42	7.243	1831	1836	1841	rBB	161	232	0.04%	0.005%
43	7.494	1911	1914	1916	rBV	162	130	0.02%	0.003%
44	7.514	1917	1920	1925	rVV	131	125	0.02%	0.003%
45	7.568	1925	1937	1954	rVV	70259	121327	21.26%	2.689%
46	7.903	2027	2041	2058	rBV	256084	433811	76.03%	9.615%
47	7.973	2058	2063	2074	rVV2	3590	5565	0.98%	0.123%
48	8.015	2074	2076	2079	rVB	230	149	0.03%	0.003%
49	8.182	2117	2128	2149	rBV	51335	84898	14.88%	1.882%
50	8.285	2156	2160	2164	rBV2	207	182	0.03%	0.004%
51	8.337	2174	2176	2181	rVB	244	184	0.03%	0.004%
52	8.362	2181	2184	2188	rBB	158	153	0.03%	0.003%
53	8.407	2191	2198	2200	rBV	171	242	0.04%	0.005%
54	8.446	2207	2210	2213	rVB	162	135	0.02%	0.003%
55	8.475	2214	2219	2223	rBV2	452	593	0.10%	0.013%
56	8.568	2246	2248	2252	rVB2	275	189	0.03%	0.004%
57	8.591	2252	2255	2258	rVB2	215	171	0.03%	0.004%
58	8.639	2258	2270	2297	rBV	167694	296558	51.97%	6.573%
59	8.845	2331	2334	2337	rBV	179	165	0.03%	0.004%
60	9.044	2393	2396	2399	rVB	174	139	0.02%	0.003%
61	9.083	2403	2408	2411	rBV	152	196	0.03%	0.004%
62	9.324	2478	2483	2486	rBV	148	198	0.03%	0.004%
63	9.420	2499	2513	2531	rBV	278172	452296	79.27%	10.024%
64	9.578	2557	2562	2565	rVB2	335	315	0.06%	0.007%
65	9.600	2566	2569	2572	rBV	154	147	0.03%	0.003%
66	9.697	2595	2599	2607	rVB2	374	458	0.08%	0.010%
67	9.841	2639	2644	2647	rBV	160	213	0.04%	0.005%
68	10.021	2696	2700	2707	rBV	198	328	0.06%	0.007%
69	10.192	2749	2753	2757	rBV	177	240	0.04%	0.005%
70	10.674	2896	2903	2908	rVB3	813	955	0.17%	0.021%
71	10.758	2917	2929	2946	rVV	198622	314680	55.15%	6.974%
72	10.825	2946	2950	2954	rVB2	199	178	0.03%	0.004%
73	10.896	2968	2972	2974	rBV2	179	155	0.03%	0.003%
74	11.095	3030	3034	3036	rBV	306	283	0.05%	0.006%
75	11.266	3083	3087	3088	rBV	144	123	0.02%	0.003%
76	11.462	3145	3148	3151	rBV	237	191	0.03%	0.004%

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Integration Parameters: LSCINT.P

Integrator: RTE
 Smoothing : OFF Filtering: 5
 Sampling : 1 Min Area: 0 % of largest Peak
 Start Thrs: 0.2 Max Peaks: 100
 Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
 Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM112921WMA.M
 Title : VOC Analysis

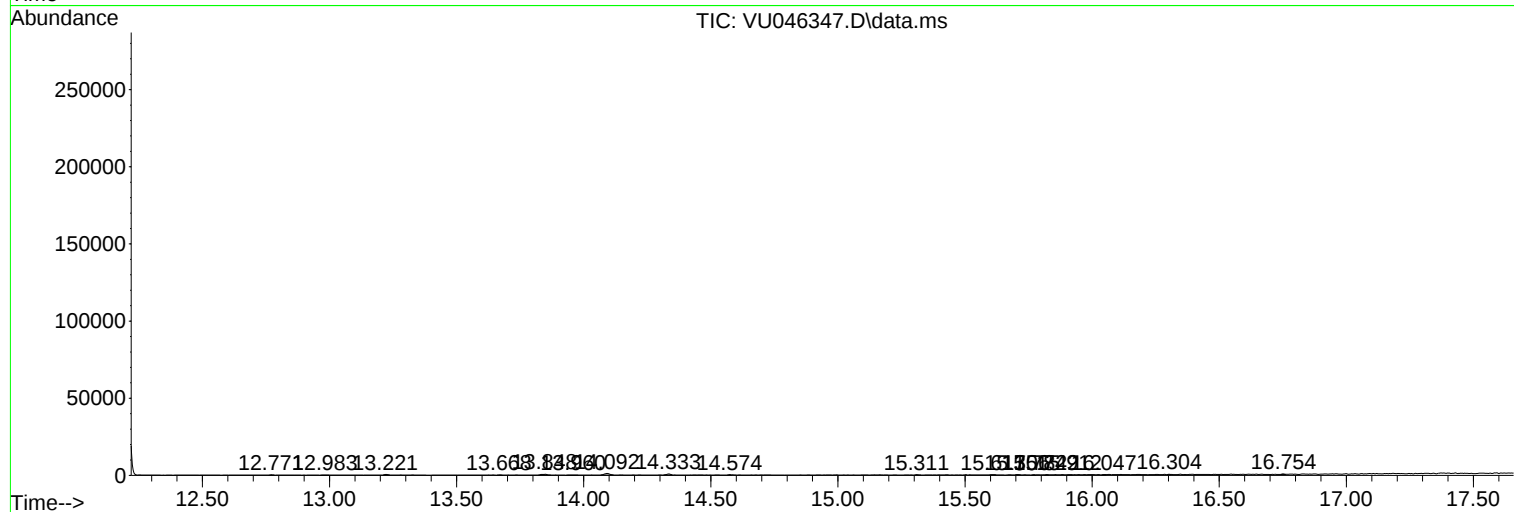
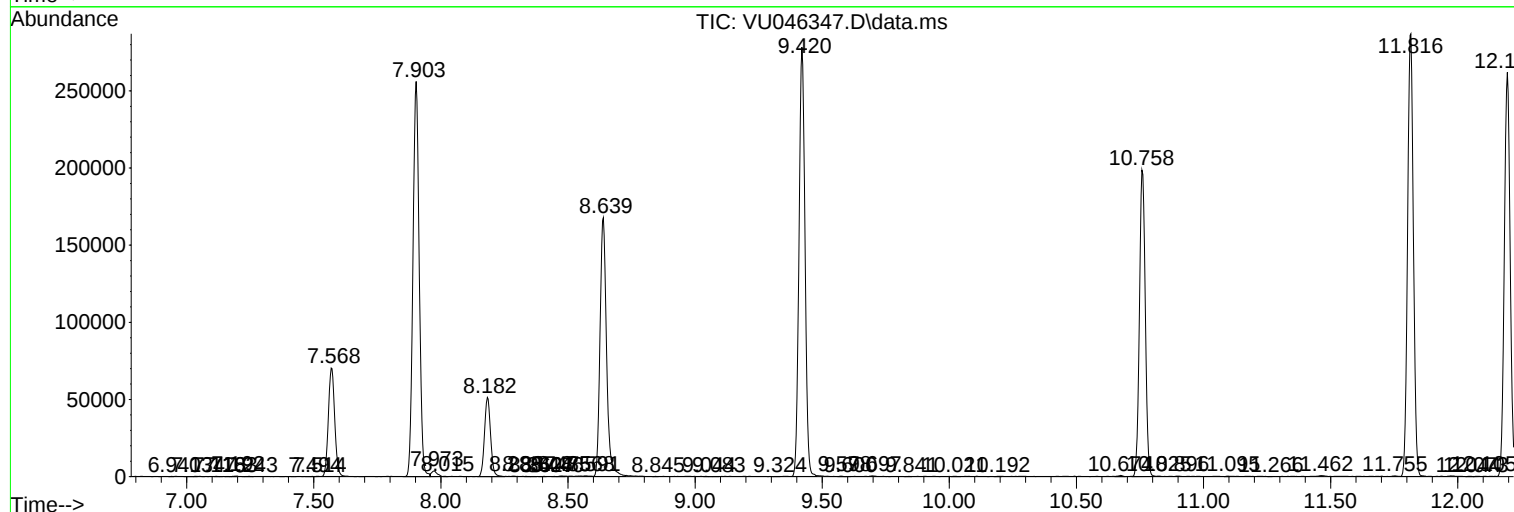
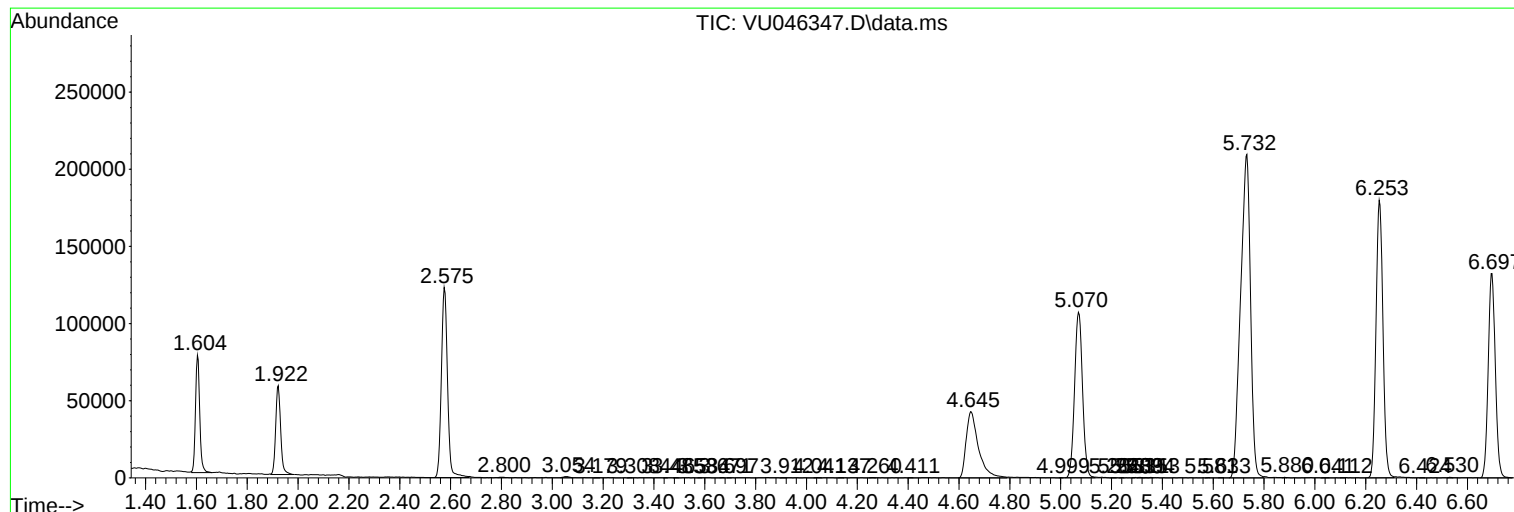
77	11.755	3235	3239	3242	rBV	284	209	0.04%	0.005%
78	11.816	3245	3258	3277	rVB	286914	450047	78.87%	9.974%
79	12.044	3326	3329	3335	rBV	190	280	0.05%	0.006%
80	12.073	3335	3338	3344	rVV	156	193	0.03%	0.004%
81	12.105	3345	3348	3352	rVV	145	124	0.02%	0.003%
82	12.195	3363	3376	3391	rVV	261891	415559	72.83%	9.210%
83	12.771	3552	3555	3559	rVB	265	184	0.03%	0.004%
84	12.983	3615	3621	3626	rBV	140	197	0.03%	0.004%
85	13.221	3692	3695	3700	rVB	416	403	0.07%	0.009%
86	13.668	3831	3834	3838	rBV	172	140	0.02%	0.003%
87	13.848	3882	3890	3897	rBV3	586	839	0.15%	0.019%
88	13.960	3916	3925	3931	rBV	137	247	0.04%	0.005%
89	14.092	3958	3966	3974	rBV	1021	1560	0.27%	0.035%
90	14.333	4035	4041	4046	rVB2	696	829	0.15%	0.018%
91	14.574	4113	4116	4118	rBV	270	152	0.03%	0.003%
92	15.311	4342	4345	4350	rVB	310	219	0.04%	0.005%
93	15.613	4434	4439	4442	rBV2	159	153	0.03%	0.003%
94	15.706	4465	4468	4472	rVV2	238	180	0.03%	0.004%
95	15.774	4485	4489	4490	rBV2	226	139	0.02%	0.003%
96	15.822	4501	4504	4506	rBV	184	130	0.02%	0.003%
97	15.912	4528	4532	4535	rBV	144	129	0.02%	0.003%
98	16.047	4571	4574	4576	rBV	214	174	0.03%	0.004%
99	16.304	4651	4654	4655	rBV2	238	142	0.02%	0.003%
100	16.754	4790	4794	4796	rBV	380	267	0.05%	0.006%

Sum of corrected areas: 4512009

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM112921WMA.M
Quant Title : VOC Analysis

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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TIC Library : C:\Database\NIST20.L
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No Library Search Compounds Detected

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TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
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